

Path Integrals and the WKB approximation in Loop Quantum Cosmology

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We follow the Feynman procedure to obtain a path integral formulation of loop quantum cosmology starting from the Hilbert space framework. Quantum geometry effects modify the weight associated with each path so that the effective measure on the space of paths is different from that used in the Wheeler-DeWitt theory. These differences introduce some conceptual subtleties in arriving at the WKB approximation. But the approximation is well defined and provides intuition for the differences between loop quantum cosmology and the Wheeler-DeWitt theory from a path integral perspective.

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I. INTRODUCTION

In loop quantum cosmology (LQC) [1, 2] quantum effects become dominant in the Planck era near the big bang and big-crunch singularities. Because of the underlying quantum geometry of loop quantum gravity (LQG), the theory inherits a repulsive force. This force is completely negligible when the curvature is less than, say, 1% of the Planck scale but then grows dramatically, overwhelming the classical gravitational attraction and causing a quantum bounce that resolves the classical singularity [3–5]. The effect is generic in the sense that it holds, for example, in absence *or* presence of a cosmological constant, anisotropies, and spatial curvature [6–11]. From a path integral viewpoint (see, e.g., [12]), on the other hand, this stark departure from classical solutions seems rather surprising at first. For, in the path integral formulation quantum effects usually become important when the action is comparable to the Planck's constant \hbar while the action along classical trajectories that originate or end in the singularity is generically very large. Thus there is conceptual tension. It is therefore desirable to understand LQC results from a path integral perspective. The goal of this paper is to fill this gap at the level of rigor that is common in the discussion of path integrals.

LQC is formulated in the Hamiltonian framework where one works with a Hilbert space and operators, appropriately taking into account the subtleties that arise because of the presence of a Hamiltonian constraint and the absence of an external time parameter. In the traditional path integral approach, on the other hand, one generally *defines* the quantum theory by integrating over the space of classical geometries, each path being weighted by

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e^{iS} where S is the Einstein Hilbert action, supplemented by suitable boundary terms [12]. These procedures then leads to the conceptual tension discussed above. To resolve it, we will return to the original derivation of path integrals [13], where Feynman began with the expressions of transition amplitudes in the Hamiltonian theory and *reformulated* them as an integral over all kinematically allowed paths. But now there is a twist: We are dealing with a constrained system without external time. In this case the analog of the transition amplitude is an *extraction amplitude* —a Green’s function which extracts physical quantum states from kinematical ones and also provides the physical inner product between them (see, e.g., [14, 15, 17]). If the theory can be deparameterized, it inherits a relational time variable and then the extraction amplitude can be re-interpreted as a transition amplitude with respect to that time [15]. Irrespective of whether this is possible, the basic object that encodes quantum dynamics is the extraction amplitude and we are led to start with its expression in LQC and cast it as a path integral. The final result will be quite similar to the traditional path integrals based on geometrodynamics [12]. However, there are also key differences. As one would expect, these emerge from the fact that since LQG is based on a quantum theory of geometry, now one cannot simply start with paths represented by smooth, classical metrics. It is precisely these differences that lead to large deviations from the classical behavior in the Planck regime near the big bang. Thus, it is possible to understand the singularity resolution of LQC also in the path integral language provided the choice of paths and the weight assigned to them —i.e., the effective measure— appropriately incorporate effects of quantum geometry. Our rewriting of the canonical theory in the path integral framework and the associated WKB approximation is also of interest in its own right as it is likely to provide new insights and tools in LQC.

In simplest models one can construct two different path integrals from the Hilbert space theory. On the one hand, one can choose to express the transition amplitude as an integral over paths in *configuration space*. On the other hand, one can consider an integral over *phase space* paths. In LQC the geometric operator corresponding to the configuration variable has a discrete spectrum. As a consequence, if one descends from the Hamiltonian theory, the construction of a configuration space path integral leads to a ‘sum over discrete histories’, as in [14–16]. This sum resembles the vertex expansion of spinfoams [18] rather than a standard path integral which features continuous paths with weights given by the exponential of a phase (i times an action). In this paper, by contrast, we will use phase space paths and arrive at a standard form of the path integral. One can then apply usual techniques as for ordinary path integrals. In particular, we will be able to carry out the saddle point evaluation of the path integral and use WKB methods.

The paper is organized as follows. We begin in Sec.II by giving a brief summary of the LQC model we wish to use. In Sec.III we derive the phase space path integral for this model. Its saddle point approximation is then studied in Sec.IV. We conclude with a summary and discussion in Sec.V. In familiar quantum mechanics the WKB approximation provides the leading term in an \hbar expansion of the transition amplitude. In Appendix A we recast that \hbar expansion to extraction amplitudes of constrained systems. This expansion provides the point of departure for the WKB approximation in Sec.IV. Finally, AppendixB recalls some technical results from [15] that are used in Sec.IV.

II. SOLVABLE LQC

We will focus on the LQC model that has been analyzed in the most detail [3–5, 21]: the $k=0$, $\Lambda=0$ Friedmann model with a massless scalar field as a source, which has the advantage of being exactly solvable [21]. However, it would not be difficult to extend this analysis to allow for a non-zero cosmological constant [6, 7], anisotropies [8, 9] or to the spatially compact $k=1$ case [11].

In the FRW models, one begins by fixing a (spatial) manifold S , topologically \mathbb{R}^3 , Cartesian coordinates x^i thereon, and a fiducial metric q_{ab}^o given by $q_{ab}^o dx^a dx^b = dx_1^2 + dx_2^2 + dx_3^2$. The physical 3-metric q_{ab} is then determined by a scale factor a ; $q_{ab} = a^2 q_{ab}^o$. For the Hamiltonian analysis one fixes a cubical fiducial cell \mathcal{V} whose volume with respect to q_{ab}^o is V_o so that its physical volume is $V = a^3 V_o$. The classical gravitational phase space will be described by the canonical pair

$$\nu = \frac{a^3 V_o}{2\pi G}, \quad b = -\frac{4\pi G}{3V_o} \frac{p_a}{a^2}, \quad (2.1)$$

where p_a is the conjugate momentum of a ; their Poisson bracket is then given by $\{\nu, b\} = -2$. The matter phase space is described by the canonical pair ϕ and p , with $\{\phi, p\} = 1$. Note *two differences from the previous LQC literature* [14, 15, 21]: there is no $\hbar\gamma$ in the definitions of ν and b and the momentum conjugate to ϕ is denoted here by p rather than $p_{(\phi)}$. The first change removes unnecessary complications in the \hbar expansions one often makes while working with path integrals while the second just simplifies notation.

In the quantum theory, the kinematical Hilbert space is a tensor product $\mathcal{H}_{\text{kin}} = \mathcal{H}_{\text{kin}}^{\text{grav}} \otimes \mathcal{H}_{\text{kin}}^{\text{matt}}$ of the gravitational and matter Hilbert spaces. Elements $\Psi(\nu)$ of $\mathcal{H}_{\text{kin}}^{\text{grav}}$ are functions of ν with support on a countable number of points and with finite norm $\|\Psi\|^2 := \sum_{\nu} |\Psi(\nu)|^2$. The matter Hilbert space is the standard one: $\mathcal{H}_{\text{kin}}^{\text{matt}} = L^2(\mathbb{R}, d\phi)$.

Thus, the kinematic quantum states of the model are functions $\Psi(\nu, \phi)$ with finite norm $\|\Psi\|^2 := \sum_{\nu} \int d\phi |\Psi(\nu, \phi)|^2$. A (generalized) orthonormal basis in \mathcal{H}_{kin} is given by $|\nu, \phi\rangle$ with

$$\langle \nu', \phi' | \nu, \phi \rangle = \delta_{\nu'\nu} \delta(\phi', \phi). \quad (2.2)$$

A notable feature of kinematics of LQC is that the normalization involves a Kronecker delta even though ν is a continuous variable at this stage. Quantum dynamics is encoded in the constraint equation,

$$-\widehat{C}\Psi(\nu, \phi) \equiv (-\widehat{p}^2 + \Theta)\Psi(\nu, \phi) = 0, \quad (2.3)$$

where $\widehat{p} = -i\hbar\partial_{\phi}$ and Θ is the positive, self-adjoint operator acting on $\mathcal{H}_{\text{kin}}^{\text{grav}}$ [22] given by

$$\Theta := \frac{3\pi G}{\ell_o^2} \left(\sqrt{|\widehat{\nu}|} \widehat{\sin \ell_o b} \sqrt{|\widehat{\nu}|} \right)^2. \quad (2.4)$$

Here ℓ_o is related to the ‘area gap’ $\Delta = 4\sqrt{3}\pi\gamma\ell_{\text{Pl}}^2$ via $\ell_o^2 = \gamma^2\Delta$, where γ is the Barbero-Immirzi parameter of LQG, $\widehat{\nu}$ acts by multiplication, and $\widehat{e^{i\ell_o b}}$ by translation: $(\widehat{e^{i\ell_o b}}\Psi)(\nu) = \Psi(\nu + 2\ell_o\hbar)$. (Again, there is a small departure from the notation used in the previous literature [14, 15, 21] in that ℓ_o^2 was set to Δ there. This change will facilitate the semi-classical considerations.) The explicit form of Θ is the following second order difference

operator

$$(\Theta\Psi)(\nu) = -\frac{3\pi G}{4\ell_o^2} \left[\sqrt{|\nu(\nu + 4\ell_o\hbar)|} |\nu + 2\ell_o\hbar| \Psi(\nu + 4\ell_o\hbar) - 2\nu^2\Psi(\nu) \right. \\ \left. + \sqrt{|\nu(\nu - 4\ell_o\hbar)|} |\nu - 2\ell_o\hbar| \Psi(\nu - 4\ell_o\hbar) \right]. \quad (2.5)$$

From (2.5) one can see that the space of solutions to the quantum constraint is naturally decomposed into sectors in which the wave functions have support on specific ‘ ν -lattices’ [4]. Furthermore these sectors are preserved by a complete set of physical observables that is of direct physical interest. Thus there is superselection and in each superselected sectors the configuration variable ν assumes discrete values. For definiteness, we will restrict ourselves to the lattice $\nu = 4n\ell_o\hbar$ where n is an integer. On this sector ν resembles the momentum variable of a particle on a circle, whence the conjugate variable b now lies in a bounded interval $(0, \pi/\ell_o)$.

Solutions to the constraint equation, as well as their inner product, can be obtained through the group averaging procedure. Given a state $|\Psi_{\text{kin}}\rangle$ in the kinematical space \mathcal{H}_{kin} , a physical state $|\Psi_{\text{phys}}\rangle$ (i.e. a solution to the constraint equation) is given by:

$$|\Psi_{\text{phys}}\rangle = \int d\alpha e^{\frac{i}{\hbar}\alpha\widehat{C}} |\Psi_{\text{kin}}\rangle \quad (2.6)$$

(see, e.g., [15]). Here, we have introduced the \hbar factor in (2.6) for later convenience. (Since the dimensions of the constraint are $[\widehat{C}] = \text{ML}^3$, α has dimensions of L^{-2} .) A Green’s function¹ for the above transformation is then given by [14, 15]

$$A(\nu_f, \phi_f; \nu_i, \phi_i) := \int d\alpha \langle \nu_f, \phi_f | e^{\frac{i}{\hbar}\alpha\widehat{C}} | \nu_i, \phi_i \rangle, \quad (2.7)$$

in terms of which (2.6) can be written as

$$\Psi_{\text{phys}}(\nu, \phi) = \sum_{\nu'} \int d\phi' A(\nu, \phi; \nu', \phi') \Psi_{\text{kin}}(\nu', \phi'). \quad (2.8)$$

In other words, A gives the matrix elements of the ‘extractor’ that extracts a physical state from every (suitably regular) kinematical one. Therefore, it will be referred to as the *extraction amplitude*.

The inner product between two physical states $|\Phi_{\text{phys}}\rangle$ and $|\Psi_{\text{phys}}\rangle$ is defined as follows. Let $|\Phi_{\text{kin}}\rangle$ and $|\Psi_{\text{kin}}\rangle$ be kinematical states such that under the extraction map defined by Eq. (2.6) they get mapped to the given physical states. The physical inner product is then defined by the action of the ‘bra’ $\langle\Phi_{\text{phys}}|$ on the ‘ket’ $|\Psi_{\text{kin}}\rangle$, or equivalently,

$$(\Phi_{\text{phys}}, \Psi_{\text{phys}}) := \langle\Phi_{\text{kin}}| \int d\alpha e^{\frac{i}{\hbar}\alpha\widehat{C}} |\Psi_{\text{kin}}\rangle \\ = \sum_{\nu, \nu'} \int d\phi d\phi' \bar{\Phi}_{\text{kin}}(\nu, \phi) A(\nu, \phi; \nu', \phi') \Psi_{\text{kin}}(\nu', \phi'). \quad (2.9)$$

¹ We will actually restrict ourselves to the ‘positive frequency part’ as in [14, 15], so that there is an implicit $\theta(\hat{p})$ factor in (2.7) where θ is the unit step function. We do not write it explicitly just to avoid unnecessary proliferation of symbols.

Thus, in the ‘timeless’ framework without any deparametrization, all the information of the quantum dynamics is encoded in the extraction amplitude $A(\nu_f, \phi_f; \nu_i, \phi_i)$. We will start by finding a path integral expression for this function.

Remark: Detailed analysis shows that ϕ is a viable relational time variable [3–5] and one can use it to deparameterize the theory. When this is done, the extraction amplitude $A(\nu_f, \phi_f; \nu_i, \phi_i)$ can also be regarded as the amplitude for a transition from ν_i at ‘time’ ϕ_i to ν_f and ‘time’ ϕ_f [15]. Even though the deparameterized theory is closer to more familiar path integrals where one also computes transition amplitudes, in the main body of this paper we will work in the timeless framework. Although the two are equivalent, the timeless framework is technically simpler because it leads to a path integral that directly involves matrix elements of Θ ; in the deparameterized framework it would involve matrix elements of $\sqrt{\Theta}$ which are much more complicated [15].

III. PHASE SPACE PATH INTEGRAL

In ordinary quantum mechanics, path integrals provide an expression for the matrix elements of the evolution operator. Feynman [13] first derived it from the canonical theory by writing the evolution as a composition of N infinitesimal ones and inserting complete basis between these infinitesimal evolution operators. He then arrived at a ‘discrete time’ path integral expression; the continuum path integral was found by taking the limit $N \rightarrow \infty$.

In the timeless framework there is no ‘evolution’ operator—all we have is the constraint equation and its solutions—and the extraction amplitude $A(\nu_f, \phi_f; \nu_i, \phi_i)$ replaces the transition amplitude. Thus, our task is to construct a path integral expression of this object. The idea is to mimic the standard Feynman construction [13] but now using the operator $e^{\frac{i}{\hbar}\alpha\hat{C}}$ that appears on the integrand of Eq. (2.7) for the ‘evolution’ operator, and then performing the α integration.

Let us be more specific. The integrand of (2.7) can be thought of as a matrix element of the fictitious evolution operator $e^{\frac{i}{\hbar}\alpha\hat{C}}$. One can regard $\alpha\hat{C}$ as playing the role of a (purely mathematical) Hamiltonian, the evolution time bring unit, i.e. $e^{\frac{i}{\hbar}\alpha\hat{C}} = e^{\frac{i}{\hbar}t\hat{H}}$ with $\hat{H} = \alpha\hat{C}$ and $t = 1$. We now decompose this fictitious evolution into N evolutions of length $\epsilon = 1/N$: $e^{\frac{i}{\hbar}t\hat{H}} = \prod_{n=1}^N e^{\frac{i}{\hbar}\epsilon\hat{H}}$. By inserting complete basis of the form $\mathbf{1} = \sum_v \int d\phi |\nu, \phi\rangle \langle \nu, \phi|$ in between each factor we get

$$\begin{aligned} \langle \nu_f, \phi_f | e^{\frac{i}{\hbar}\alpha\hat{C}} | \nu_i, \phi_i \rangle &= \sum_{\nu_{N-1}, \dots, \nu_1} \int d\phi_{N-1} \dots d\phi_1 \langle \nu_N, \phi_N | e^{\frac{i}{\hbar}\epsilon\alpha\hat{C}} | \nu_{N-1}, \phi_{N-1} \rangle \dots \\ &\dots \langle \nu_1, \phi_1 | e^{\frac{i}{\hbar}\epsilon\alpha\hat{C}} | \nu_0, \phi_0 \rangle, \end{aligned} \quad (3.1)$$

where $\langle \nu_N, \phi_N | \equiv \langle \nu_f, \phi_f |$ and $| \nu_0, \phi_0 \rangle \equiv | \nu_i, \phi_i \rangle$.

Let us concentrate on the n -th term appearing in (3.1). Notice that since the constraint is a sum of two commuting pieces that act separately on $\mathcal{H}_{\text{kin}}^{\text{matt}}$ and $\mathcal{H}_{\text{kin}}^{\text{grav}}$, one has the following factorization:

$$\langle \nu_{n+1}, \phi_{n+1} | e^{\frac{i}{\hbar}\epsilon\alpha\hat{C}} | \nu_n, \phi_n \rangle = \langle \phi_{n+1} | e^{\frac{i}{\hbar}\epsilon\alpha\hat{p}^2} | \phi_n \rangle \langle \nu_{n+1} | e^{-\frac{i}{\hbar}\epsilon\alpha\Theta} | \nu_n \rangle. \quad (3.2)$$

The scalar field factor can easily be evaluated by inserting a complete basis in p ,

$$\langle \phi_{n+1} | e^{\frac{i}{\hbar} \epsilon \alpha \hat{p}^2} | \phi_n \rangle = \int \frac{dp_n}{2\pi} e^{\frac{i}{\hbar} p_n (\phi_{n+1} - \phi_n) + \frac{i}{\hbar} \epsilon \alpha p_n^2}. \quad (3.3)$$

The gravitational factor in (3.2) is less trivial to compute. As usual in the path integral construction, we will take $N \gg 1$ ($\epsilon \equiv 1/N \ll 1$) and use an expansion in ϵ to compute this term:

$$\langle \nu_{n+1} | e^{-\frac{i}{\hbar} \epsilon \alpha \Theta} | \nu_n \rangle = \delta_{\nu_{n+1}, \nu_n} - \frac{i}{\hbar} \epsilon \alpha \langle \nu_{n+1} | \Theta | \nu_n \rangle + \mathcal{O}(\epsilon^2), \quad (3.4)$$

where the matrix element of Θ can be obtained from Eq. (2.5) and is given by

$$\langle \nu_{n+1} | \Theta | \nu_n \rangle = -\frac{3\pi G}{4\ell_o^2} \sqrt{|\nu_n \nu_{n+1}|} \frac{(\nu_n + \nu_{n+1})}{2} (\delta_{\nu_{n+1}, \nu_n + 4\ell_o} - 2\delta_{\nu_{n+1}, \nu_n} + \delta_{\nu_{n+1}, \nu_n - 4\ell_o}). \quad (3.5)$$

(There are several equivalent ways of writing this matrix element. Here we chose one that is symmetric in ν_n and ν_{n+1} .) As in usual path integral constructions, we now bring-in b , the conjugate variable to ν . This can be done through the identity

$$\delta_{\nu', \nu} = \frac{\ell_o}{\pi} \int_0^{\pi/\ell_o} db e^{-\frac{i}{2\hbar} b(\nu' - \nu)}, \quad (3.6)$$

which, when used to rewrite the Kronecker deltas appearing in Eqs. (3.4) and (3.5), leads to the following expression for (3.4):

$$\begin{aligned} \langle \nu_{n+1} | e^{-\frac{i}{\hbar} \epsilon \alpha \hat{\Theta}} | \nu_n \rangle &= \frac{\ell_o}{\pi} \int_0^{\pi/\ell_o} db_{n+1} e^{-\frac{i}{\hbar} b_{n+1} (\nu_{n+1} - \nu_n)/2} \left[1 - \frac{i}{\hbar} \epsilon \alpha \frac{3\pi G}{\ell_o^2} \sqrt{\nu_n \nu_{n+1}} \frac{\nu_n + \nu_{n+1}}{2} \sin^2(\ell_o b_{n+1}) \right] + \mathcal{O}(\epsilon^2) \\ &= \frac{\ell_o}{\pi} \int_0^{\pi/\ell_o} db_{n+1} e^{-\frac{i}{\hbar} b_{n+1} (\nu_{n+1} - \nu_n)/2 - i\epsilon \alpha \frac{3\pi G}{\ell_o^2} \sqrt{\nu_n \nu_{n+1}} \frac{\nu_n + \nu_{n+1}}{2} \sin^2(\ell_o b_{n+1})} + \mathcal{O}(\epsilon^2). \end{aligned} \quad (3.7)$$

By combining (3.2), (3.3) and (3.7), the amplitude (3.1) takes the form

$$\begin{aligned} \langle \nu_f, \phi_f | e^{i\alpha \hat{C}} | \nu_i, \phi_i \rangle &= \sum_{\nu_{N-1}, \dots, \nu_1} \left(\frac{\ell_o}{\pi} \right)^N \int db_N \dots db_1 \int d\phi_{N-1} \dots d\phi_1 \times \\ &\quad \left(\frac{1}{2\pi} \right)^N \int dp_N \dots dp_1 e^{\frac{i}{\hbar} S_N} + \mathcal{O}(\epsilon^2), \end{aligned} \quad (3.8)$$

where

$$\begin{aligned} S_N = \epsilon \sum_{n=0}^{N-1} \left[p_{n+1} \frac{\phi_{n+1} - \phi_n}{\epsilon} - \frac{b_{n+1}}{2} \frac{\nu_{n+1} - \nu_n}{\epsilon} \right. \\ \left. + \alpha \left(p_n^2 - \frac{3\pi G}{\ell_o^2} \sqrt{\nu_n \nu_{n+1}} \frac{\nu_n + \nu_{n+1}}{2} \sin^2(\ell_o b_{n+1}) \right) \right] \end{aligned} \quad (3.9)$$

can be heuristically regarded as a ‘discrete-time action’. Thus, following Feynman, we have obtained an approximate expression of the extraction amplitude as a sum over phase space paths, approximation becoming better and better as ϵ shrinks and N grows.

Already, before taking the $N \rightarrow \infty$ limit, we can see two important differences from the more familiar path integrals. First, whereas in the classical theory the variables ν and b can

take all real values, our paths in ν take only discrete values and the paths in b are bounded; the allowed values of ν and b are dictated by spectrum of the corresponding operators on the superselected sector we began with. Second, we find that the action is not just a discretization of the classical action, but includes quantum gravity corrections (namely, the so-called ‘holonomy type corrections’ encoded here in the sin term). What is the origin of these differences? After all, we just mimicked the Feynman construction [13] to arrive at (3.9) starting from the Hamiltonian theory. Recall however, that Feynman began with the standard Schrödinger representation of quantum mechanics. In LQG, because of the underlying diffeomorphism invariance the analogous representation is not viable [19]. This difference descends to LQC where kinematics is based on a ‘polymer’ representation that is unitarily *inequivalent* to the Schrödinger representation [20]. In the polymer representation, the quantum constraint operator of the Wheeler-DeWitt theory—which would have been analogous to the Hamiltonian operator Feynman used—fails to be well-defined. Defining a viable constraint operator on the kinematical Hilbert space of LQC requires an appropriate incorporation of quantum geometry underlying LQG [5]. And this is directly responsible for the two key differences mentioned above.

The final step in the path integral construction involves taking the limit $N \rightarrow \infty$. In this limit one typically performs the substitutions $\epsilon \sum_{n=0}^N \rightarrow \int d\tau$, $(\phi_{n+1} - \phi_n)/\epsilon \rightarrow d\phi/d\tau$, etc, to obtain a continuum (in time) action. However, due to the discrete nature of ν , it is not possible to interpret the $(\nu_{n+1} - \nu_n)/\epsilon$ as a derivative. Therefore, we are led to carry out an ‘integrating by parts,’ rewriting this term as

$$\epsilon \sum_{n=0}^{N-1} \left[-\frac{b_{n+1}}{2} \frac{\nu_{n+1} - \nu_n}{\epsilon} \right] = \epsilon \sum_{n=0}^{N-1} \left[\frac{\nu_n}{2} \frac{b_{n+1} - b_n}{\epsilon} \right] + \frac{1}{2}(b_1 \nu_0 - b_N \nu_N). \quad (3.10)$$

Now the formal limit can be carried out at the same level of precision as is common in path integrals and one obtains

$$A(\nu_f, \phi_f; \nu_i, \phi_i) = \int d\alpha \int [\mathcal{D}\nu_q(\tau)] [\mathcal{D}b_q(\tau)] [\mathcal{D}p(\tau)] [\mathcal{D}\phi(\tau)] e^{\frac{i}{\hbar} \bar{S}}, \quad (3.11)$$

where

$$\bar{S} = \int_0^1 d\tau \left(p\dot{\phi} + \frac{1}{2}\nu\dot{b} - \alpha \left(p^2 - 3\pi G\nu^2 \frac{\sin^2 \ell_o b}{\ell_o^2} \right) \right) - \frac{1}{2}(\nu_f b_f - \nu_i b_i) \quad (3.12)$$

and the subscript q emphasizes the fact that we have taken the formal limit of a sum that included only ‘quantum paths’ in the geometrical sector. Thus, the integral is over paths $\nu(\tau)$ taking only the values $\nu = 4n\ell_o\hbar$ and the paths $b(\tau)$ take values in the range $(0, \pi/\ell_o)$. Notice that the classically singular paths where b is divergent are *excluded*, which reflects the fact that the quantum dynamics is free of singularities. However, precisely because of the unusual restriction on the domain of integration, this path integral is not of the usual type. The path integral (3.11) actually resembles the ‘sum over histories’ of [15], where one sums over the same family of ν -paths. Indeed, by performing the b_q integral in (3.11) one can recover the sum over histories expansion of [15].

But it turns out that we can express this path integral also in a more familiar form using a clever trick from path integral framework for a particle in a circle [23]. The trick is to use the identity

$$\sum_{m \in \mathbb{Z}} \int_0^{2\pi} d\theta f(\theta, m) e^{im\theta} = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} d\theta f(\theta, x) e^{ix\theta} \quad (3.13)$$

which holds for any continuous $f(\theta, x)$ with a 2π period in θ to convert the discrete sum over m to a continuous integral over x . Let us then return to the finite N or ‘discrete-time’ path integral (3.8) and use this identity. Then, we are led to rewrite each sum over ν_n and integral over b_n appearing in (3.8) as

$$\frac{\pi}{\ell_o} \sum_{\nu_n} \int_0^{\pi/\ell_o} db_n \dots \rightarrow \int_{-\infty}^{\infty} d\nu_n \int_{-\infty}^{\infty} db_n \dots \quad (3.14)$$

(this is done for $n = 1, \dots, N-1$; the integral over b_N remains unchanged). The allowed paths now take value over the whole classical phase space: ν is no longer restricted to be discrete nor is b required to be bounded. As in standard path integral discussions, it is then possible to take the formal limit $N \rightarrow \infty$. We obtain²

$$A(\nu_f, \phi_f; \nu_i, \phi_i) = \int d\alpha \int [\mathcal{D}\nu(\tau)] [\mathcal{D}b(\tau)] [\mathcal{D}p(\tau)] [\mathcal{D}\phi(\tau)] e^{\frac{i}{\hbar} S}, \quad (3.15)$$

where

$$S = \int_0^1 d\tau \left(p\dot{\phi} - \frac{1}{2}b\dot{\nu} - \alpha \left(p^2 - 3\pi G\nu^2 \frac{\sin^2 \ell_o b}{\ell_o^2} \right) \right). \quad (3.16)$$

While this is the same action as before, *one now integrates over all trajectories in the classical phase space as in usual path integrals*. In particular, the trajectories that make the action stationary lie in the domain of integration (which, by contrast, were not included in the ‘quantum paths’ of the previous path integral). We can therefore use all the standard techniques such as the saddle point approximation. Thus, while they are (formally) equivalent, this second form (3.15) of the path integral is much more convenient in practice, particularly to address the issues we began with in Sec.I. This is the path integral form of the extraction amplitude we were seeking.

Since we now integrate over all paths in the classical phase space, in particular, the paths are allowed to go through the classical singularity. How can then we see the singularity resolution in this setting? The answer is that the paths are not weighted by the standard FRW action but by a ‘polymerized’ version of it which still retains the memory of the quantum geometry underlying the Hamiltonian theory. As we will see, this action is such that a path going through the classical singularity has negligible contribution whereas bouncing trajectories give the dominant contribution.

Remark: There are other systems in which the passage from the Hamiltonian quantum theory to a path integral results in an action that has \hbar -corrections. Perhaps the simplest example is that of a non-relativistic particle on a curved Riemannian manifold for which the standard Hamiltonian operator is simply $\hat{H} = -(\hbar^2/2m)g^{ab}\nabla_a\nabla_b$. Quantum dynamics generated by this \hat{H} can be recast in the path integral form following the Feynman procedure [13]. The transition amplitude is then given by [25]

$$\langle q, t | q', t' \rangle = \int \mathcal{D}[q(\tau)] e^{\frac{i}{\hbar} S} \quad (3.17)$$

² Note that the integral over α is an ordinary one variable integral. It can nevertheless be reinterpreted as an integral over *all* possible values $\alpha(\tau)$ together with the gauge fixing condition $d\alpha/d\tau = 0$. Doing so allows one to rewrite the path integral with any other gauge fixing condition; see for instance [24].

with

$$S = \int d\tau \left(\frac{m}{2} g_{ab} \dot{q}^a \dot{q}^b + \frac{\hbar^2}{12m} R \right) \quad (3.18)$$

where R is the scalar curvature of the metric g_{ab} . Extrema of this action are not the geodesics one obtains in the classical theory but rather particle trajectories in a \hbar -dependent potential. The two sets of trajectories can be qualitative different.

IV. SADDLE POINT APPROXIMATION

As we saw in Sec.II, the extraction amplitude encodes the entire content of quantum dynamics. However, in practice, it is difficult to work with the series (3.8) or evaluate its limit (3.15). In quantum mechanics and quantum field theory the steepest descent approximation is a powerful practical tool to calculate leading contributions to the transition amplitude in an \hbar expansion. In particular, this approximation provides the much needed intuition on when quantum corrections are dynamically important and when they are not. In Appendix A we recast this \hbar expansion in a form suitable for the extraction amplitude of constrained systems. We will now use those results to obtain the leading term using a saddle point approximation.

In this approximation, the extraction amplitude (3.15) is given by

$$A(\nu_f, \phi_f; \nu_i, \phi_i) \sim (\det \delta^2 S|_0)^{-1/2} e^{\frac{i}{\hbar} S|_0}. \quad (4.1)$$

Here $S|_0$ is the action evaluated along the trajectory extremizing the action with initial and final configuration points fixed. For given initial and final points, there exist in general two trajectories joining them, one with positive and the other with negative p values. As pointed out in Sec.II, following the logic spelled out in [15] here we restrict ourselves to the ‘positive frequency’ branch, and so only the $p > 0$ trajectory gets picked. We will evaluate the phase factor in Sec.IV A. The prefactor $(\det \delta^2 S|_0)^{-1/2}$ represents a formal infinite dimensional determinant which we will evaluate in Sec.IV B. In Sec.IV C we compare the resulting approximate amplitude to the exact one, computed numerically.

Before proceeding with these calculations, we would like to point out a conceptual subtlety. In ordinary quantum mechanics, the steepest descent approximation provides the leading term in the transition amplitude in an \hbar expansion. In our case, the action S that features in the path integral (3.15) itself depends on \hbar through $\ell_o \sim \sqrt{\gamma^3 \hbar G}$, while the \hbar expansion of Appendix A assumes that the action does not change as \hbar tends to zero. Therefore, to directly apply the result of Appendix A, now we have to take the limit $\hbar \rightarrow 0$ while keeping ℓ_o fixed. Hence we will obtain the leading term in the extraction amplitude in the approximation $\hbar \rightarrow 0$, $\gamma \rightarrow \infty$ keeping $\gamma^3 \hbar$ fixed. To emphasize this subtlety, *we will use inverted commas, as in ‘classical limit’ and ‘semi-classical approximation’ while referring to this limit.* Let us briefly explore the meaning of this limit. In classical general relativity, $\gamma \rightarrow \infty$ corresponds to ignoring the new term in the Holst action for general relativity, in comparison with the standard Palatini term. What about the ‘semi-classical’ approximation? Eigenvalues of the volume operator are given by $(8\pi G \ell_o \hbar) n$ where n is a non-negative integer. Therefore, in the ‘semi-classical limit’ the spacing between consecutive eigenvalues goes to zero and ν effectively becomes continuous as one would expect. Finally, states that are relevant in this limit have large n , just as quantum states of a rigid rotor that are relevant in the semi-classical limit have large j .

A. The Hamilton-Jacobi function $S|_0$

To calculate the $S|_0$ term, we need to solve the equations of motion obtained from the action (3.16), then evaluate the action along those trajectories, and finally express the result in terms of the given initial and final points. The (positive frequency) trajectories which solve the equations of motion can be written in terms of two integration constants, ν_B and ϕ_B , as

$$\nu(\phi) = \nu_B \cosh(\sqrt{12\pi G}(\phi - \phi_B)), \quad (4.2)$$

$$b(\phi) = \frac{2 \operatorname{sign}(\nu_B)}{\ell_o} \tan^{-1}(e^{-\sqrt{12\pi G}(\phi - \phi_B)}). \quad (4.3)$$

These solutions have several interesting features.

- (i) As seen from the cosh dependence of the volume, these trajectories represent bouncing universes, with ϕ_B and ν_B giving the scalar field and volume values at the bounce point. The minimum volume ν_B is related with the scalar field momentum p by $|\nu_B| = 2\ell_o p / \sqrt{12\pi G}$. Note that if ν_B is positive (resp. negative), then $\nu(\phi)$ remains positive (resp. negative) for all ϕ . For concreteness we will focus on trajectories with positive ν_B .
- (ii) $\nu(\phi)$ can vanish only on the trajectory with $\nu_B = 0$ i.e., $\nu(\phi) = 0$ for all ϕ . Thus if we begin with the initial state $\nu_i \neq 0, \phi_i$, there is no (real) ‘classical’ trajectory at all with $\nu_f = 0$ for any value of ϕ_f .
- (iii) Whereas in general relativity *all* trajectories begin at the big-bang—they all tend to $\nu = 0$ as $\phi \rightarrow -\infty$ —it is obvious from (4.2) that all our trajectories tend to $\nu \rightarrow \infty$ in this limit (except for the trajectory $\nu(\phi) = 0 \forall \phi$).
- (iv) Recall that in full LQC, states which are sharply peaked at a low curvature configuration for large values of ϕ remain sharply peaked on certain ‘effective trajectories’ for all ϕ [5]. These are among solutions (4.3).
- (v) The relation between ν and ϕ given in Eq. (4.2) coincides with the expression for the expectation value of the volume operator at a given scalar field value ϕ in *any* quantum state of LQC [21].

Evaluation of the action along these solutions can be greatly simplified if one integrates by parts the term $-\int_0^1 d\tau \frac{1}{2} b \dot{\nu}$ in (3.16). Then, using the equations of motion, the terms $\frac{1}{2} \dot{b} \nu$ and $p \dot{\phi}$ cancel each other and the action evaluated along the solutions is just given by only the boundary term,

$$S|_0 = \frac{1}{2} (\nu_i b_i - \nu_f b_f). \quad (4.4)$$

To express $S|_0$ in terms of initial and final configuration variables, we need to solve for the constants ν_B and ϕ_B in terms of $\nu_f, \phi_f; \nu_i, \phi_i$. Without loss of generality we can take $\phi_i = 0$ and $\phi_f = \varphi$ (by setting $\varphi = \phi_f - \phi_i$ at the end, one recovers the general case). Then we are led to solve the equations

$$\nu_i = \nu_B \cosh(-\sqrt{12\pi G} \phi_B) \quad (4.5)$$

$$\nu_f = \nu_B \cosh(\sqrt{12\pi G}(\varphi - \phi_B)), \quad (4.6)$$

for ν_B and ϕ_B in terms of the initial and final data:

$$e^{\sqrt{12\pi G}\phi_B} = \sqrt{\frac{e^{\sqrt{12\pi G}\varphi} - \nu_f/\nu_i}{-e^{-\sqrt{12\pi G}\varphi} + \nu_f/\nu_i}} \quad (4.7)$$

$$\nu_B = \frac{\nu_i}{|\sinh(\sqrt{12\pi G}\varphi)|} \sqrt{\left(e^{\sqrt{12\pi G}\varphi} - \frac{\nu_f}{\nu_i}\right) \left(-e^{-\sqrt{12\pi G}\varphi} + \frac{\nu_f}{\nu_i}\right)}. \quad (4.8)$$

Clearly, ν_B, ϕ_B are real for any given initial configuration (ν_i, ϕ_i) if and only if the final configuration satisfies

$$e^{-\sqrt{12\pi G}|\varphi|} < \frac{\nu_f}{\nu_i} < e^{\sqrt{12\pi G}|\varphi|}. \quad (4.9)$$

This is the necessary and sufficient condition for the existence of real trajectories. Let us first focus on the ‘classically’ allowed region (4.9). Using (4.3) to express b_i and b_f appearing in (4.4) in terms of the initial and final data $(\nu_f, \phi_f; \nu_i, \phi_i)$ we obtain the desired expression of the Hamilton-Jacobi function:

$$S|_0 = \frac{\nu_i}{\ell_o} \tan^{-1} \left(\sqrt{\frac{e^{\sqrt{12\pi G}\varphi} - \nu_f/\nu_i}{-e^{-\sqrt{12\pi G}\varphi} + \nu_f/\nu_i}} \right) - \frac{\nu_f}{\ell_o} \tan^{-1} \left(e^{-\sqrt{12\pi G}\varphi} \sqrt{\frac{e^{\sqrt{12\pi G}\varphi} - \nu_f/\nu_i}{-e^{-\sqrt{12\pi G}\varphi} + \nu_f/\nu_i}} \right), \quad (4.10)$$

where $\varphi = \phi_f - \phi_i$. The ‘classically’ allowed region consists of the upper and lower quarters in Fig. 1. For ν_f, ϕ_f in these two quarters, S_0 is real and thus the amplitude (4.1) has an oscillatory behavior. Outside these regions the action becomes imaginary and one gets an exponentially suppressed amplitude. Thus, the situation is analogous to that in quantum mechanics.

For completeness, let us now discuss the case where the final point lies in the ‘classically’ forbidden region, this is to say the situation where the boundary data satisfy

$$\frac{\nu_f}{\nu_i} < e^{-\sqrt{12\pi G}|\varphi|} \quad \text{or} \quad \frac{\nu_f}{\nu_i} > e^{\sqrt{12\pi G}|\varphi|}. \quad (4.11)$$

For concreteness let ν_i be positive as in Fig.1 but now there is no restriction on the sign of ν_f . To find extrema of the action that join the initial and final configurations satisfying (4.11), we can follow the semi-classical procedure used to calculate tunneling amplitudes in familiar systems and allow paths with imaginary momenta. Let us define

$$\tilde{b} = ib, \quad \tilde{p} = ip, \quad \tilde{\alpha} = i\alpha, \quad \tilde{S} = iS. \quad (4.12)$$

Eq. (3.16) then implies

$$\tilde{S} = \int d\tau \left(\tilde{p}\dot{\phi} - \frac{1}{2}\tilde{b}\dot{\nu} + \tilde{\alpha} \left(\tilde{p}^2 - 3\pi G\nu^2 \frac{\sinh^2 \ell_o \tilde{b}}{\ell_o^2} \right) \right). \quad (4.13)$$

We now consider the case when the tilde quantities are real and compute the stationary trajectories of \tilde{S} . The ‘positive frequency’ (i.e. $\tilde{p} > 0$) trajectories are parameterized by two

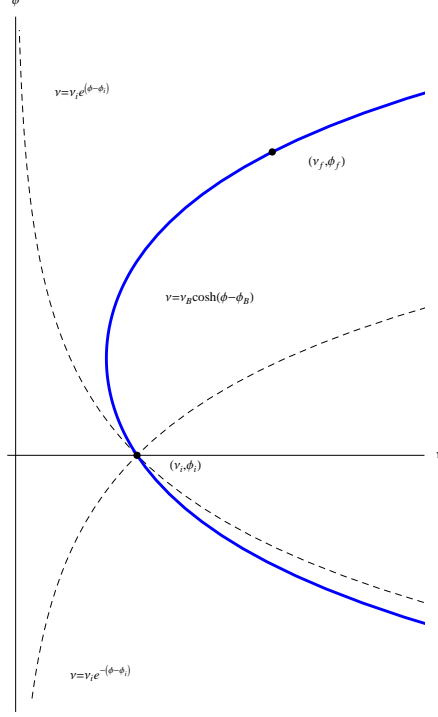


FIG. 1: For fixed (ν_i, ϕ_i) , the (dashed) curves $\nu_f = \nu_i e^{\pm\sqrt{12\pi G}(\phi_f - \phi_i)}$ divide the (ν_f, ϕ_f) plane into four regions. For a final point in the upper or lower quarter, there always exists a real trajectory joining the given initial and final points (as exemplified by the thick line). If the final point lies on the left or right quarter, there is no real solution matching the two points. The action becomes imaginary and one gets an exponentially suppressed amplitude.

integrations constants, ν_o and ϕ_o , and take the form

$$\nu(\phi) = \nu_o \sinh(\sqrt{12\pi G}(\phi - \phi_o)), \quad (4.14)$$

$$\tilde{b}(\phi) = \frac{2 \operatorname{sign}(\nu_o)}{\ell_o} \tanh^{-1}(e^{-\sqrt{12\pi G}|\phi - \phi_o|}). \quad (4.15)$$

They represent universes that go through a singularity at $\phi = \phi_o$, where the volume vanishes and \tilde{b} diverges. As in the ‘classically’ allowed region we have $|\nu_o| = 2\ell_o \tilde{p}/\sqrt{12\pi G}$. In terms of the initial and final data, the integration constants are

$$e^{\sqrt{12\pi G}\phi_o} = \sqrt{\frac{e^{\sqrt{12\pi G}\varphi} - \nu_f/\nu_i}{e^{-\sqrt{12\pi G}\varphi} - \nu_f/\nu_i}} \quad (4.16)$$

$$\nu_o = \frac{|\nu_i| \operatorname{sign}(\nu_f - \nu_i)}{\sinh(\sqrt{12\pi G}\varphi)} \sqrt{\left(e^{\sqrt{12\pi G}\varphi} - \frac{\nu_f}{\nu_i}\right) \left(e^{-\sqrt{12\pi G}\varphi} - \frac{\nu_f}{\nu_i}\right)}, \quad (4.17)$$

which, as expected, take real values in the ‘forbidden’ region (4.11). The action can then be evaluated as before. Although now the paths encounter a divergence in \tilde{b} , the integral (4.13) is convergent and given by the tilde version of (4.4). (Moreover, the product $\nu(\phi)\tilde{b}(\phi)$ is always finite and vanishes at $\phi = \phi_o$.) For the case when $\varphi > 0$ and $\nu_f/\nu_i < e^{-\sqrt{12\pi G}\varphi}$ the

result is

$$\tilde{S}|_0 = \frac{\nu_i}{\ell_o} \tanh^{-1} \left(\sqrt{\frac{e^{-\sqrt{12\pi G}\varphi} - \nu_f/\nu_i}{e^{\sqrt{12\pi G}\varphi} - \nu_f/\nu_i}} \right) - \frac{\nu_f}{\ell_o} \tanh^{-1} \left(e^{\sqrt{12\pi G}\varphi} \sqrt{\frac{e^{-\sqrt{12\pi G}\varphi} - \nu_f/\nu_i}{e^{\sqrt{12\pi G}\varphi} - \nu_f/\nu_i}} \right). \quad (4.18)$$

Similar expressions hold for other regions. For instance, in the $\varphi > 0$, $\nu_f/\nu_i > e^{\sqrt{12\pi G}\varphi}$ case the action takes the same form, except that the arguments of the \tanh^{-1} functions are the reciprocals of the ones appearing in (4.18).

In all cases, $\tilde{S}|_0$ is negative; the extraction amplitude is exponentially suppressed for paths in the ‘classically forbidden’ regions. But as we approach the dashed curves marking the boundary of the ‘classically’ allowed and forbidden regions, the action \tilde{S} goes to zero. In particular then, from Fig.1 it may appear that for any given ν_i there is a significant probability of reaching the singularity $\nu_f = 0$ for large $\varphi = \phi_f - \phi_i$. However, as is common in more familiar systems, the steepest descent approximation also becomes poor in a neighborhood of the dashed curves! Indeed, we know from full LQC that (in the deparameterized framework) the expectation value of $|\hat{\nu}|$ tends to *infinity* for large φ . More generally, plots of the exact extraction amplitudes in Sec.IV C will show that the amplitude is always suppressed in the classically forbidden regions. Thus, while the steepest descent approximation provides much physical insight, it is by no means a substitute for the full quantum theory.

B. $\det \delta^2 S|_0$ and the WKB approximation

To compute the amplitude $(\det \delta^2 S|_0)^{-1/2}$, one would need to perform some regularization in order to deal with the infinite dimensional determinant. This can be done in ordinary quantum mechanics or field theory, and should as well be doable here. We will however take a different route and calculate this factor by means of the WKB approximation [26, 27].

Note that the extraction amplitude $A(\nu_f, \phi_f; \nu_i, \phi_i)$ can be thought of as a physical state if one takes the initial data as fixed parameters and the final data as arguments of the wavefunction: the family of states

$$\Psi_{\nu_i, \phi_i}(\nu_f, \phi_f) := A(\nu_f, \phi_f; \nu_i, \phi_i), \quad (4.19)$$

parameterized by ν_i and ϕ_i satisfy the constraint equation

$$\hat{C} \Psi_{\nu_i, \phi_i} = 0. \quad (4.20)$$

The \hbar expansions underlying the desired WKB approximation are discussed in Appendix A. We begin with the ansatz for the physical state:

$$\Psi_{\nu_i, \phi_i}(\nu_f, \phi_f) = a(\nu_f, \phi_f; \nu_i, \phi_i) e^{\frac{i}{\hbar} W(\nu_f, \phi_f; \nu_i, \phi_i) + \mathcal{O}(\hbar)}. \quad (4.21)$$

Following the procedure of Appendix A, the imposition of the constraint equation (4.20) to zeroth and first order in \hbar leads to the following equations for a and W :

$$C(\nu_f, \phi_f, \partial_{\nu_f} W, \partial_{\phi_f} W) = 0, \quad \text{and} \quad \mathcal{L}_X a = 0 \quad (4.22)$$

where

$$C(\nu_f, \phi_f, b_f, p_f) = p_f^2 - 3\pi G \frac{\sin^2 \ell_o b_f}{\ell_o^2} \nu_f^2$$

is the ‘effective constraint’, and

$$X = \left. \frac{\partial C}{\partial p_f} \right|_{p_f = \partial_{q_f} W} \frac{\partial}{\partial q_f}$$

is the vector field on configuration space $q_f = (\nu_f, \phi_f)$ obtained from the Hamiltonian vector field of the constraint.

The first equation is the Hamilton-Jacobi equation and, as expected, one can check that $S|_0$ given by (4.10) solves it. The amplitude a is determined by the second equation together with the condition

$$a(\nu_i, \phi_i; \nu_f, \phi_f) = a(\nu_f, \phi_f; \nu_i, \phi_i) \quad (4.23)$$

which follows from the fact that $\bar{\Psi}_{\nu_i, \phi_i}(\nu_f, \phi_f) = \Psi_{\nu_f, \phi_f}(\nu_i, \phi_i)$:

$$a = |\nu_i^2 (e^{\sqrt{12\pi G}\varphi} - \frac{\nu_f}{\nu_i}) (-e^{-\sqrt{12\pi G}\varphi} + \frac{\nu_f}{\nu_i})|^{-1/4}. \quad (4.24)$$

This is the factor we identify with $(\det \delta^2 S|_0)^{-1/2}$. Note that this quantity diverges at $\nu_f = \nu_i e^{\pm \sqrt{12\pi G}\varphi}$ (dashed lines in Fig. 1) where the amplitude goes from oscillatory to exponential decay behavior. Thus, the WKB approximation can be valid only away from the dashed lines. This simply mirrors what happens in the WKB approximation in ordinary quantum mechanics.

To summarize, we have succeeded in finding a saddle point approximation of the path integral as in equation (4.1). The determinant factor was not calculated directly but by matching with the terms of a WKB expansion. Therefore, we will call the resulting approximate extraction amplitude A^{WKB} :

$$A^{\text{WKB}}(\nu_f, \phi_f; \nu_i, \phi_i) := a e^{\frac{i}{\hbar} S|_0}, \quad (4.25)$$

where a is given by Eq. (4.24), $S|_0$ by Eq. (4.10) and as before $\varphi = \phi_f - \phi_i$. We now proceed to numerically compare this approximate amplitude with the exact one.

C. Comparison with exact solution

One of the advantages of the model under study is its solvability [21]. In particular, it is possible to obtain a closed form expression of the extraction amplitude $A(\nu_f, \phi_f; \nu_i, \phi_i)$ [15]. This is displayed in Appendix B. We calculated the exact solution numerically and compared it with the saddle point approximation obtained in Sec.IV B. We found that there is a good agreement away from the dashed lines of Fig. 1 which mark the transition between the ‘classically’ allowed region to the ‘classically’ forbidden one. Along the dashed line, however, the WKB amplitude diverges and the approximation fails badly just as in ordinary quantum mechanics.

We illustrate these results in figures 2, 3 and 4. In the first two figures we plot of the real parts of the exact and WKB amplitudes as a function of ν_f and ϕ_f respectively, for

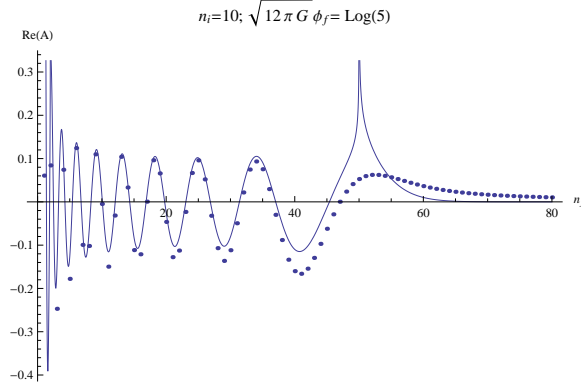


FIG. 2: Real parts of the exact and WKB amplitudes are plotted as a function of the final volume $n_f := \nu_f/4\ell_o\hbar$. The exact amplitude (dots) has support on the ‘lattice’ $(\nu_f - \nu_i)/4\ell_o\hbar \in \mathbb{Z}$. At $n_f = n_i e^{\sqrt{12\pi G}(\phi_f - \phi_i)} = 50$ there is the transition from oscillatory to exponential behavior, and the WKB amplitude (solid line) diverges. (It also diverges at $n_f = n_i e^{-\sqrt{12\pi G}(\phi_f - \phi_i)} = 2$.) Here, ϕ_i, ν_i and ϕ_f are kept fixed: $\phi_i = 0$, $n_i := \nu_i/4\ell_o\hbar = 10$ and $\sqrt{12\pi G}\phi_f = \log 5$.

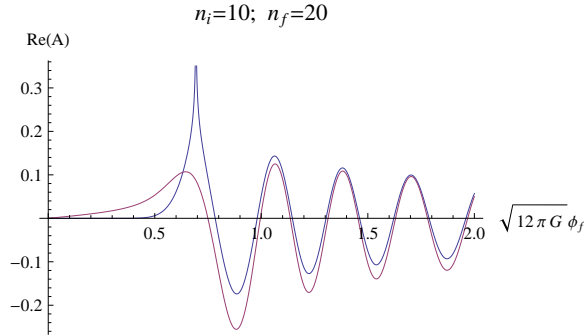


FIG. 3: Real parts of the exact and WKB amplitudes are plotted as a function of the final scalar field ϕ_f (dots and solid lines, respectively). Here ϕ_i, ν_i and ν_f are kept fixed: $\phi_i = 0, n_i := \nu_i/4\ell_o\hbar = 10$ and $n_f := \nu_f/4\ell_o\hbar = 20$. The WKB solution is the curve diverging at $\sqrt{12\pi G}\phi_f = \log(\nu_f/\nu_i) = \log 2$.

fixed values of the remaining variables. The exact amplitude shows a sudden transition from oscillatory to decaying behavior. If one had access only to the exact result, this behavior would have seemed rather puzzling. The WKB approximation provides a physical understanding of this behavior. Thus, not only does the WKB approximation reproduce the qualitative behavior of the exact extraction amplitude away from the dashed lines of Fig.1, but it anticipates that the dashed lines mark a boundary between two quite different behaviors of the exact answer and provides a physical understanding of this difference.

What can we say regarding the regime of validity of the saddle point approximation? From the path integral perspective, we expect it to be valid whenever $S/\hbar \gg 1$. From Eq. (4.10), we see that $S|_0$ scales with the volume times a coefficient which can be interpreted as measuring the departure from the dashed lines $\nu_f = \nu_i e^{\pm\sqrt{12\pi G}|\varphi|}$. At these lines $S|_0 = 0$ and, as we have just seen, the approximation totally breaks down. As we depart from these

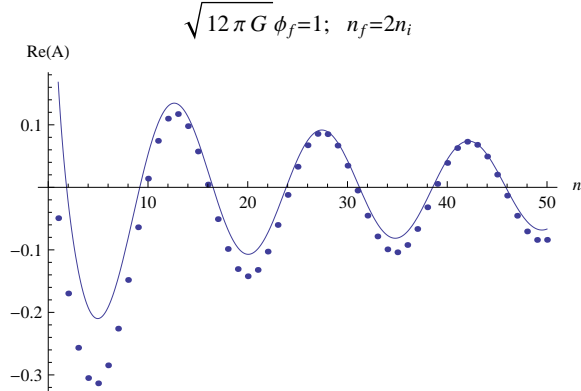


FIG. 4: Comparison of the exact and WKB amplitudes for initial and final configurations with $\nu_f = 2\nu_i$ as a function of $n_i := \nu_i/4\ell_o\hbar$. As n_i increases, the WKB solution (continuous line) becomes closer to the exact solution (dots). (The distance between the amplitudes oscillates, but overall it decreases.) This calculation was done for $\phi_i = 0$ and $\phi_f = 1/\sqrt{12\pi G}$.

lines, $S|_0$ takes a nonzero value, and its scale is given by the initial and final volume. For instance, if we keep the ratio ν_f/ν_i fixed, the action grows linearly with ν_i and we expect the approximation to improve as ν_i increases. This behavior is indeed observed, an example of which is display in Figure 4. Thus, the standard expectations on the validity of the WKB approximation are all borne out.

V. DISCUSSION

For constrained quantum systems, the extraction amplitude encodes full quantum dynamics: It enables one to extract physical quantum states from (suitably regular) kinematical ones *and* define the physical scalar product between them. In this paper we considered a solvable model in LQC. Following Feynman, we began with the expression of the extraction amplitude $A(\nu_f, \phi_f; \nu_i, \phi_i)$ in the Hilbert space framework and obtained two equivalent forms of a phase space path integral for it. In the first, one is led to integrate over paths that are very different from those one might have expected from the Wheeler-DeWitt theory: The integral is taken over *quantum paths* defined by the spectrum of the operators related to the phase space variables. However, by a clever trick from the quantum theory of a particle on a circle [23], this path integral could be reduced to one over standard classical paths. This form is better suited for semiclassical considerations and is also closer to that used in the Wheeler-DeWitt theory. However in *neither* form is the weight associated with a path given by the Einstein-Hilbert action. Instead, it is given by an action that includes quantum geometry corrections. This is the key difference from the Wheeler-DeWitt theory. Note that such a change of action in the transition from the Hamiltonian quantum theory to a path integral can occur already in much simpler systems. For example, for a particle moving on a Riemannian manifold, dynamics generated by the *standard* Hamiltonian operator, $\hat{H} = -(\hbar^2/2m) g^{ab} \nabla_a \nabla_b$, is correctly captured in the path integral framework only if one adds to the classical action an \hbar dependent term that depends on the scalar curvature of the Riemannian metric [25].

From the path integral perspective, these differences are directly responsible for the absence of singularities in LQC, i.e., for the resolution of the apparent tension we began our discussion with in Sec.I. In the first form of the path integral, the classically singular paths are not contained in the range of integration since the paths in b are bounded above while in the classical singularity $b = \infty$. Furthermore the action is no longer the classical action. In the second form of the path integral, the domain of integration does include singular paths. But now the fact that the action is corrected by quantum geometry effects becomes crucial. Indeed, in this case the equations of motion can be obtained explicitly by varying the action. These equations and their solutions describe bouncing cosmologies which are characteristic of the singularity resolution in LQC. Thus the exact results on singularity resolution in LQC are in complete harmony with the path integral intuition, once one realizes that the action that descends from the Hamiltonian theory includes quantum geometry corrections. Furthermore, because we have an additional constant in the theory —the Barbero-Immirzi parameter— it is meaningful to consider \hbar expansions while retaining quantum geometry effects. This is achieved by sharpening the precise manner in which the limit is taken: $\hbar \rightarrow 0$, $\gamma \rightarrow \infty$ such that $\hbar\gamma^3 = \text{const.}$ This \hbar expansion enables us to introduce the WKB approximation which helps one understand features of the exact amplitude, e.g., the oscillatory versus damping behavior that occurs as one varies the final configuration (ν_f, ϕ_f) keeping the initial configuration (ν_i, ϕ_i) fixed. It also provides an ‘explanation’ of the surprising effectiveness of the effective equations [28] in LQC from a path integral framework.

Thus, from the LQC perspective, it would be incorrect to simply define the theory starting with smooth metrics and matter fields and assigning to each path the weight that comes from the Einstein Hilbert action because this procedure completely ignores the quantum nature of the underlying Riemannian geometry. For a satisfactory treatment of ultraviolet issues such as the singularity resolution, it is crucial that the calculation retains appropriate memory of this quantum nature. This viewpoint can be traced back to full LQG and spinfoam models. In full LQG, quantum geometry is an essential feature already of *kinematics*. It is then not surprising that in spinfoams the histories that one sums over are *quantum geometries* (captured in appropriate, colored 2-complexes). The weight that is assigned to each history is motivated by the Einstein-Hilbert action but does not descend *directly* from it, e.g. via a discretization procedure. Rather, one begins with the action of a constrained BF theory which is classically equivalent with the Einstein Hilbert action but then incorporates the (simplicity) constraint using considerations from quantum geometry (quantum tetrahedron, representation theory and interpretation of the Casimirs as eigenvalues of geometric operators). Thus, the situation is parallel to the first form of the path integral we obtained in this paper. In LQC we were fortunate in that the integral over quantum paths could be recast into an integral over all paths in the classical phase space. This enabled us to carry out the steepest descent approximation and develop physical intuition for the qualitative properties of the exact extraction amplitude. A similar reformulation of spinfoams of the full theory appears to be difficult. But if it could somehow be achieved, one would have a powerful tool both to probe semi-classical aspects of full quantum gravity and to develop valuable intuition for the ultraviolet properties of the theory. In particular, the resulting quantum geometry corrections to the full Einstein-Hilbert action would bring the difference between spin foams and perturbative path integrals into sharp focus.

Acknowledgments

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Appendix A: WKB approximation for constrained systems

Let us consider a system with phase space \mathbb{R}^{2n} and a single constraint $C(q, p) = 0$, to be thought of as the Hamiltonian constraint. We will assume that the $C(q, p)$ can be written as a Taylor expansion in the p , as is the case for a large class of physically interesting systems.

The kinematic Hilbert space is $L^2(\mathbb{R}^n)$ of normalizable wave functions $\Psi(q) \equiv \Psi(q^1, \dots, q^n)$. The elementary operators are the usual \hat{q}^j and \hat{p}_j which act by multiplication and derivation respectively:

$$\hat{q}^j \Psi(q) = q^j \Psi(q) \quad (\text{A1})$$

$$\hat{p}_j \Psi(q) = -i\hbar \frac{\partial \Psi}{\partial q^j}(q). \quad (\text{A2})$$

The physical states are then solutions to the quantum constraint:

$$\hat{C} \Psi = 0, \quad (\text{A3})$$

where \hat{C} is an operator analog of $C(q, p)$, obtained by replacing q, p with \hat{q}^j and \hat{p}_j with a suitable choice of factor ordering. As is standard in the group averaging procedure, we will assume that \hat{C} is self-adjoint. For unconstrained systems, the WKB ansatz provides approximate solutions to the Schrödinger equation. In this Appendix we will extend that method to obtain approximate solutions of (A3) where, again, \hbar plays the role of small parameter governing the expansion. As one might expect, the main idea is to write both \hat{C} and Ψ in (A3) as expansions in \hbar , and to collect terms having the same \hbar power. Let us now explicitly calculate the zeroth and first order terms.

The construction is as follows. First, the constraint operator \hat{C} is written as a sum of ‘normal ordered’ operators, in which all \hat{q} ’s appear to the left of the \hat{p} ’s:

$$\hat{C} = \sum_{n=0}^{\infty} (\hbar/i)^n C_n \left(\overset{\text{L}}{\hat{q}}, \overset{\text{R}}{\hat{p}} \right). \quad (\text{A4})$$

Here the C_n ’s are functions on the classical phase space—for instance, C_0 will typically be the classical constraint function—which are now ‘evaluated’ on the operators \hat{q} and \hat{p} according to the ‘normal ordered’ prescription indicated by the superscripts. Second, the unknown state $\Psi(q)$ is written as the exponential

$$\Psi(q) = e^{\frac{i}{\hbar} S(q)} \quad (\text{A5})$$

where the exponent is written as a power series in \hbar :

$$S(q) = \sum_{n=0}^{\infty} (\hbar/i)^n S_n(q). \quad (\text{A6})$$

Since $C(q, p)$ is assumed to admit a Taylor expansion in the p , so do $C_n(q, p)$. Imposition of the quantum constraint (A3) now leads to the following zeroth and first order equations:

$$C_0(q, \partial_q S_0) = 0, \quad (\text{A7})$$

$$\frac{1}{2} \frac{\partial^2 C_0}{\partial p_i \partial p_j} \Big|_{p=\partial_q S_0} \frac{\partial^2 S_0}{\partial q^i \partial q^j} + \frac{\partial C_0}{\partial p_i} \Big|_{p=\partial_q S_0} \frac{\partial S_1}{\partial q^i} + C_1(q, \partial_q S_0) = 0 \quad (\text{A8})$$

The zeroth order equation (A7) can be recognized as the Hamilton-Jacobi equation. The first order one, (A8), can be rewritten as follows. If we use the fact that \widehat{C} is self-adjoint, the condition $\widehat{C}^\dagger = \widehat{C}$, when applied to (A4) implies

$$C_1 = \frac{1}{2} \frac{\partial^2 C_0}{\partial q^j \partial p_j}. \quad (\text{A9})$$

Using (A9), and writing $a(q) := e^{S_1(q)}$, Eq. (A8) can be written as a derivative of the function a along the vector field

$$X := \frac{\partial C_0}{\partial p_j} \Big|_{p=\partial_q S_0} \frac{\partial}{\partial q^j} \quad (\text{A10})$$

as

$$X(a) + \frac{1}{2} a \operatorname{div} X = 0. \quad (\text{A11})$$

The divergence term in (A11) suggest one to interpret a and $\Psi \sim a e^{\frac{i}{\hbar} S_0}$ as half densities on \mathbb{R}^n . Then (A11) is just the Lie derivative of a along X :

$$\text{Eq. (A8)} \iff \mathcal{L}_X a = 0. \quad (\text{A12})$$

These are the equations used in Sec. IV B.

Appendix B: Exact Amplitude

In Sec. IV C we compared the exact extraction amplitude with the WKB approximation. In this Appendix we recall from [15] the expression that was used in the numerical evaluation of the exact amplitude.

The first step in the calculation is to find the eigenvectors of Θ . They are given by $|k\pm\rangle$, with $k > 0$, satisfying the eigenvalue equation

$$\Theta|k\pm\rangle = 12\pi G k^2 \hbar^2 |k\pm\rangle. \quad (\text{B1})$$

These vectors are not normalized; the decomposition of the identity reads

$$\mathbf{I} = \int_0^\infty \frac{dk}{2\pi k \sinh(\pi k)} (|k+\rangle\langle k+| + |k-\rangle\langle k-|). \quad (\text{B2})$$

In terms of the ‘volume basis’ $|4n\ell_o\hbar\rangle$ used in the main body of this paper, the vectors $|k\pm\rangle$ are given by

$$\langle 4n\ell_o\hbar|k\pm\rangle = \begin{cases} \sqrt{4|n|\pi ik} P_{\pm n}(k) & \pm n \geq 0 \\ 0 & \pm n < 0 \end{cases}, \quad (\text{B3})$$

where $P_n(k)$ is the following $(2n-1)$ -degree polynomial in k :

$$P_n(k) := \frac{1}{ik(2n)!} \left. \frac{d^{2n}}{ds^{2n}} \right|_{s=0} \left(\frac{1-s}{1+s} \right)^{ik} = \sum_{m=0}^{2n} \frac{1}{m!(2n-m)!} \prod_{l=1}^{2n-1} (ik+m-l). \quad (\text{B4})$$

We are now ready to present the expression of the extraction amplitude. For this, it is convenient to work in the deparameterized framework. In [15] it was shown that the extraction amplitude in the timeless framework coincides with the transition amplitude of the deparameterized theory:

$$A(\nu_f, \phi_f; \nu_i, \phi_i) = \langle \nu_f | e^{\frac{i}{\hbar} \sqrt{\Theta}(\phi_f - \phi_i)} | \nu_i \rangle. \quad (\text{B5})$$

Let us take $\nu_i = 4\ell_o\hbar n_i$ and $\nu_f = 4\ell_o\hbar n_f$ with n_i and n_f positive integers, and define $t := \sqrt{12\pi G}(\phi_f - \phi_i)$.

By inserting the complete basis (B2) in the right hand side of (B5), we obtain

$$A(\nu_f, \phi_f; \nu_i, \phi_i) = -2\sqrt{n_i n_f} \int_0^\infty \frac{dk}{\sinh(\pi k)} P_{n_f}(k) P_{n_i}(k) k e^{ikt} \quad (\text{B6})$$

$$= -2\sqrt{n_i n_f} P_{n_f}(-i\partial_t) P_{n_i}(-i\partial_t) \int_0^\infty \frac{dk}{\sinh(\pi k)} k e^{ikt} \quad (\text{B7})$$

$$= -\frac{\sqrt{n_i n_f}}{\pi^2} P_{n_f}(-i\partial_t) P_{n_i}(-i\partial_t) \psi^{(1)}(1/2 - i\frac{t}{2\pi}) \quad (\text{B8})$$

where $\psi^{(1)}(z) = d \log \Gamma(z)/dz$, and $\Gamma(z) = (z-1)!$ is the Gamma function.

This last expression (B8) was the one used to numerically compute the exact extraction amplitude for the plots in Sec. IV C.

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